

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103019\
 Data File : BF117621.D
 Acq On : 30 Oct 2019 13:46
 Operator : JU
 Sample : K5539-19
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 165-84-(0-1)

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.351	552	555	577	rBV	428433	670594	84.52%	9.500%
2	6.381	727	730	747	rBV	554710	778384	98.10%	11.027%
3	6.504	747	751	764	rVB	827648	793440	100.00%	11.240%
4	6.728	786	789	803	rVB	215078	201538	25.40%	2.855%
5	6.881	812	815	830	rBV	596218	539167	67.95%	7.638%
6	7.292	882	885	904	rBV	337317	441877	55.69%	6.260%
7	8.010	1004	1007	1026	rBV	197155	251296	31.67%	3.560%
8	9.080	1185	1189	1203	rBV	748513	725923	91.49%	10.284%
9	9.480	1254	1257	1271	rBV	57761	68612	8.65%	0.972%
10	9.757	1301	1304	1320	rBV	255638	278043	35.04%	3.939%
11	10.557	1437	1440	1456	rBV	315463	371562	46.83%	5.264%
12	11.251	1554	1558	1567	rBV	219077	257064	32.40%	3.642%
13	11.710	1633	1636	1640	rBV2	6709	9292	1.17%	0.132%
14	11.774	1644	1647	1655	rVB3	33462	37728	4.75%	0.534%
15	12.468	1762	1765	1774	rBV	37028	40224	5.07%	0.570%
16	12.563	1778	1781	1789	rBV3	4756	9156	1.15%	0.130%
17	12.698	1799	1804	1811	rVB	32980	38116	4.80%	0.540%
18	12.827	1822	1826	1833	rBV	634694	540187	68.08%	7.653%
19	13.027	1854	1860	1862	rBV3	6992	10491	1.32%	0.149%
20	13.733	1976	1980	1991	rBV2	48072	96365	12.15%	1.365%
21	13.892	2003	2007	2011	rBV	220068	248142	31.27%	3.515%
22	14.286	2071	2074	2078	rBV4	7022	11229	1.42%	0.159%
23	14.345	2081	2084	2086	rBV2	18057	16593	2.09%	0.235%
24	14.380	2086	2090	2093	rBV6	7824	12965	1.63%	0.184%
25	14.639	2131	2134	2137	rBV2	23248	21055	2.65%	0.298%
26	14.709	2142	2146	2151	rVB	68299	63869	8.05%	0.905%
27	14.927	2180	2183	2185	rBV2	19859	23713	2.99%	0.336%
28	14.957	2185	2188	2192	rVB4	38295	45523	5.74%	0.645%
29	15.215	2229	2232	2237	rBV3	10817	14415	1.82%	0.204%
30	15.280	2240	2243	2245	rBV	11213	12006	1.51%	0.170%
31	15.333	2245	2252	2257	rVB	169399	235370	29.66%	3.334%
32	15.715	2313	2317	2321	rVB2	25137	29091	3.67%	0.412%
33	16.180	2393	2396	2401	rVB5	11176	15982	2.01%	0.226%
34	16.798	2494	2501	2510	rVB3	70522	141757	17.87%	2.008%

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Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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35	17.368	2595	2598	2603	rVB7	5359	8065	1.02%	0.114%
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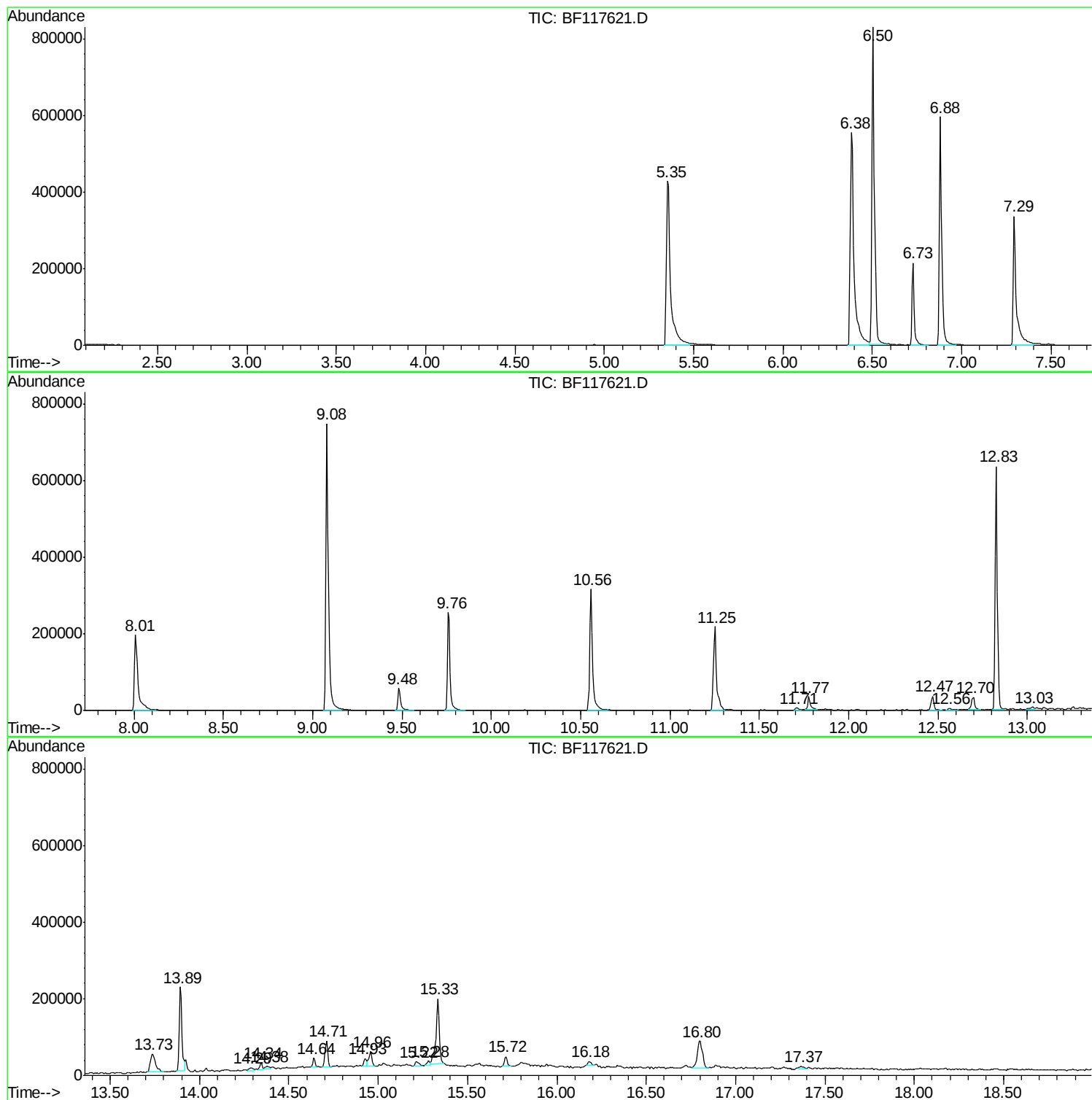
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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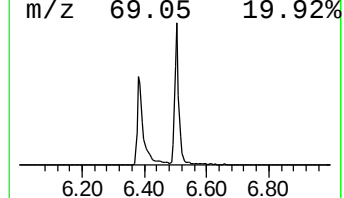
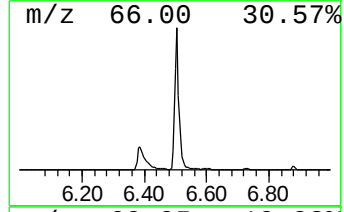
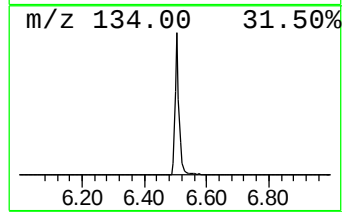
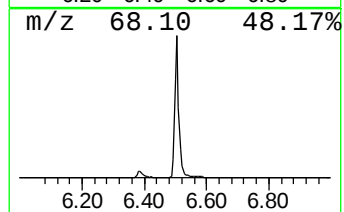
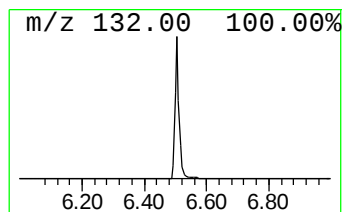
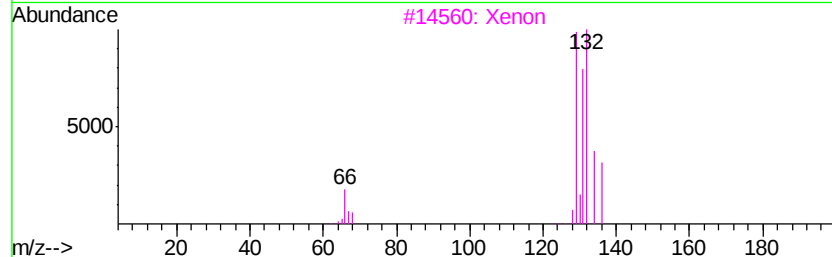
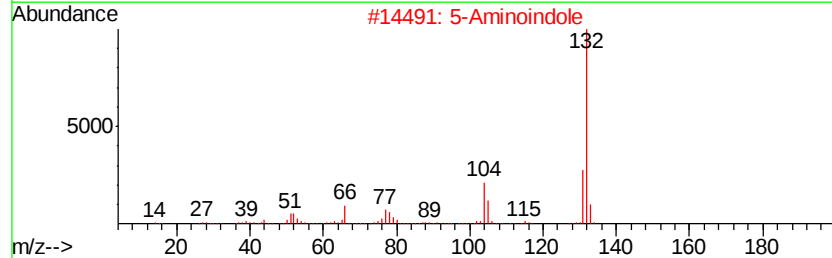
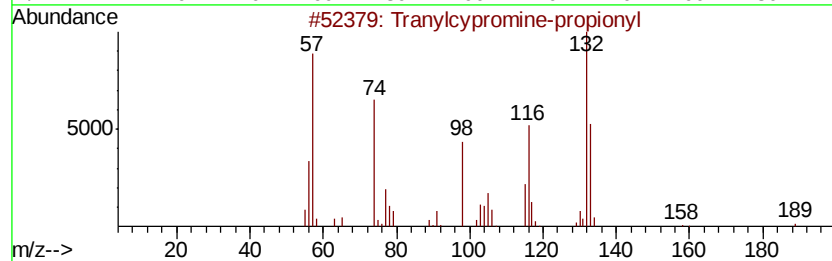
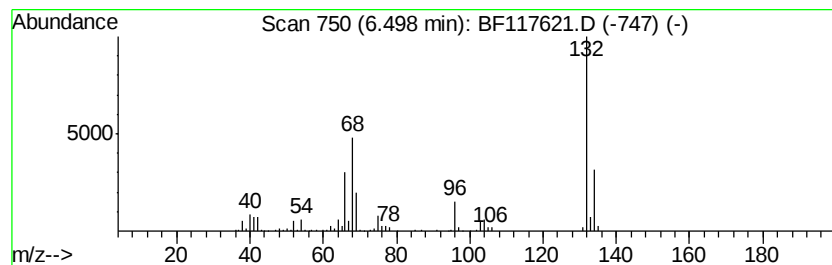
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	78.74 ng	793440	1,4-Dichlorobenzene-d4	6.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Xenon	132	Xe	007440-63-3	9
4			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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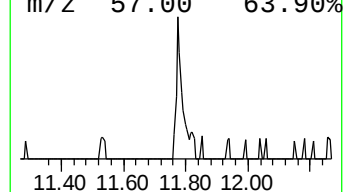
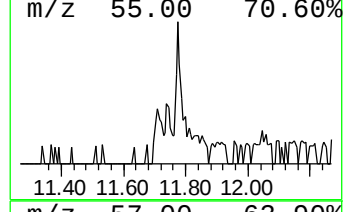
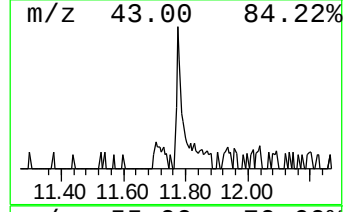
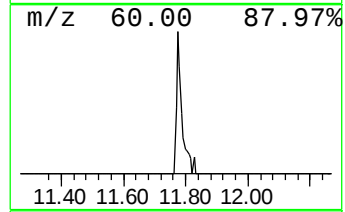
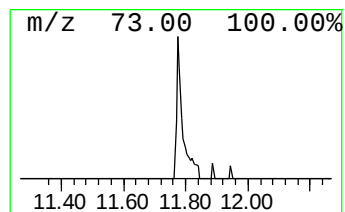
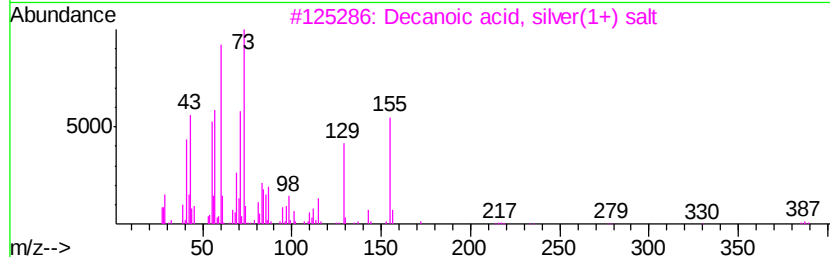
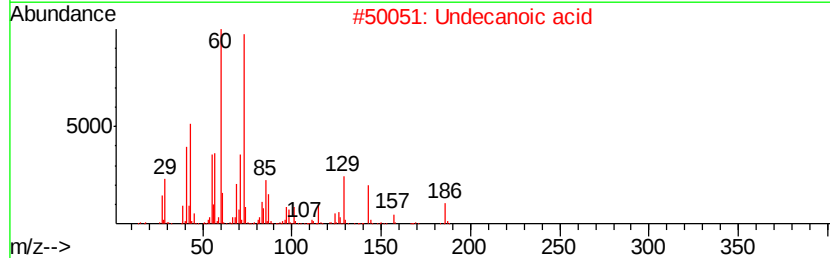
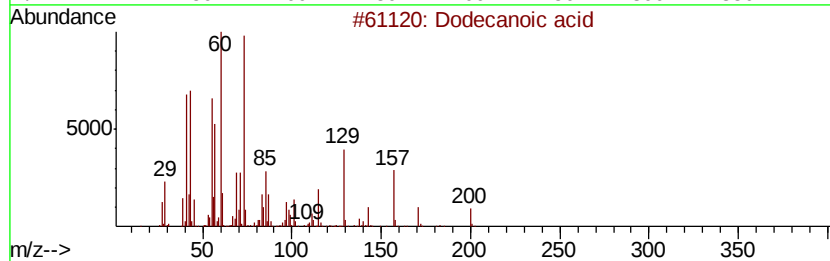
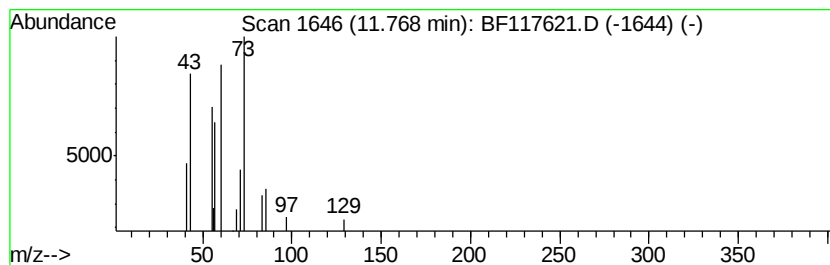
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Dodecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	2.94 ng	37728	Phenanthrene-d10	11.25

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	59
2			Undecanoic acid	186	C11H22O2	000112-37-8	53
3			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	53
4			n-Decanoic acid	172	C10H20O2	000334-48-5	43
5			.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	27



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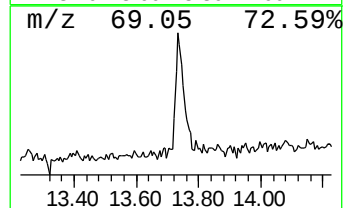
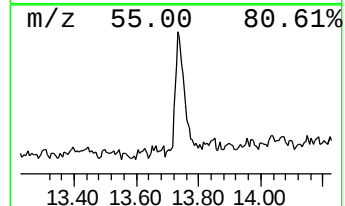
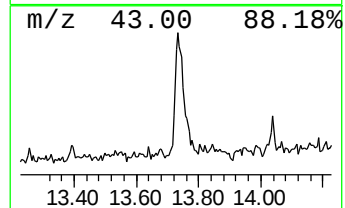
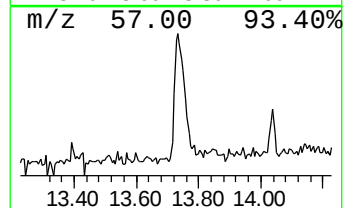
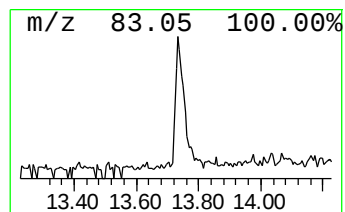
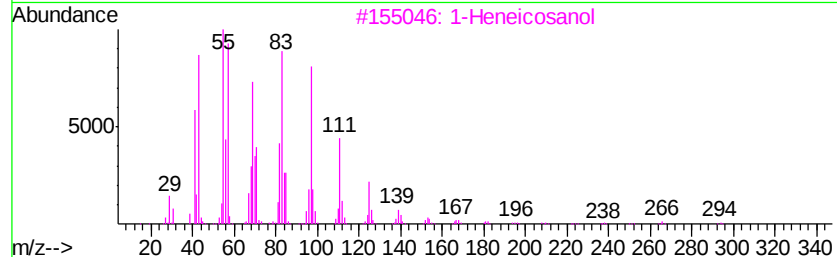
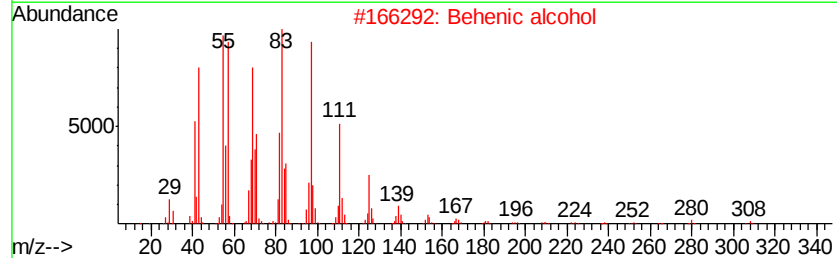
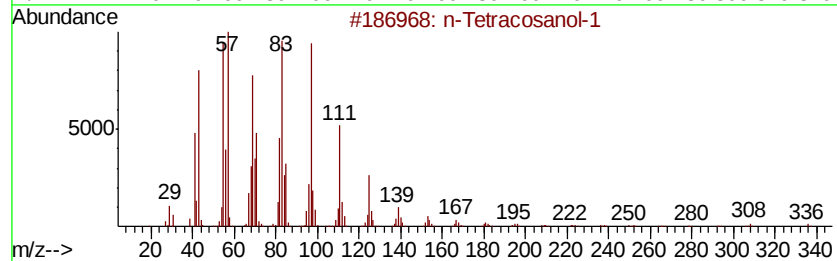
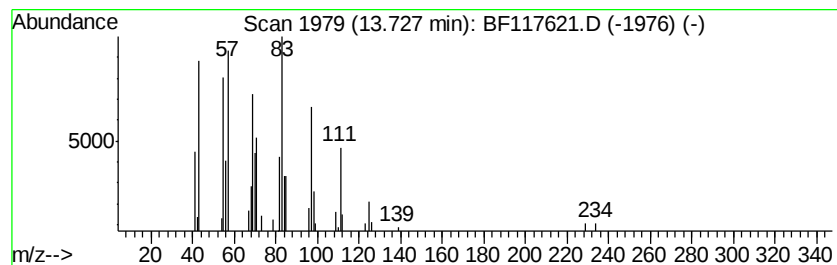
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 n-Tetracosanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	7.77 ng	96365	Chrysene-d12	13.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Tetracosanol-1	354	C24H50O	000506-51-4	95
2		Behenic alcohol	326	C22H46O	000661-19-8	94
3		1-Heneicosanol	312	C21H44O	015594-90-8	94
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	94
5		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91



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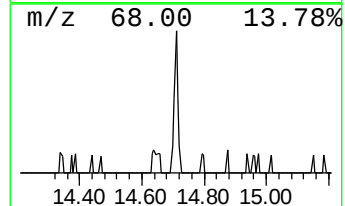
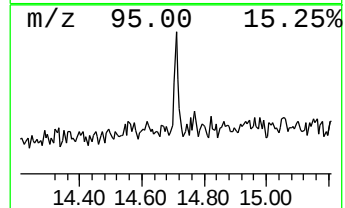
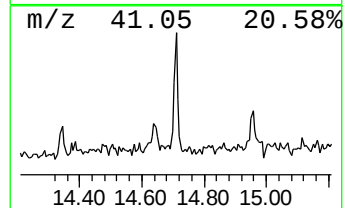
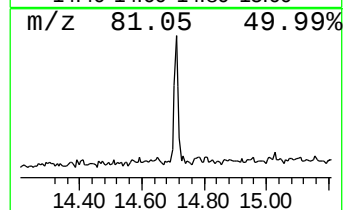
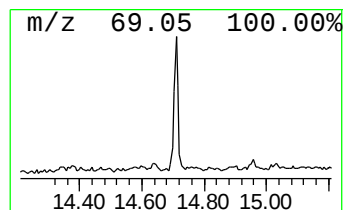
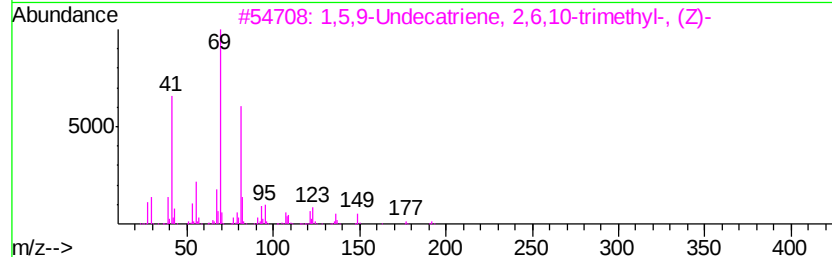
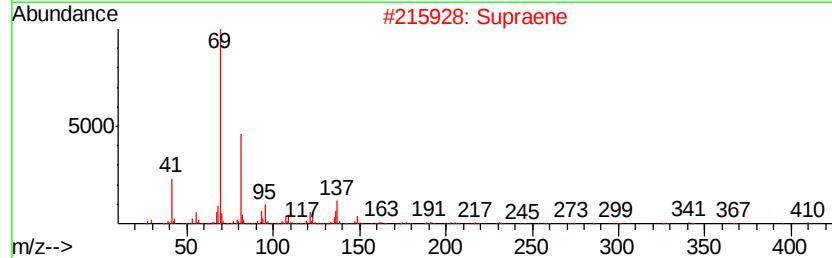
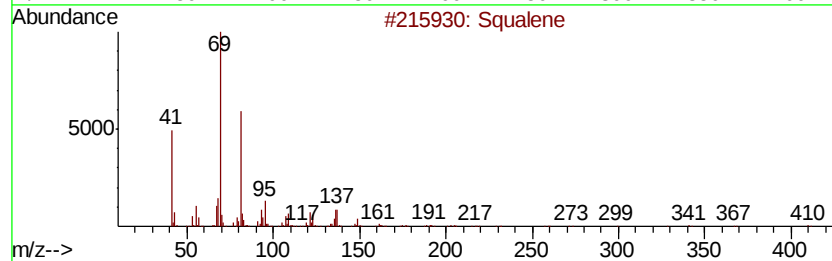
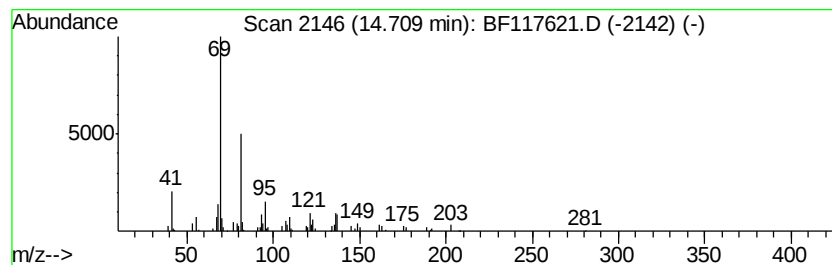
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	5.43 ng	63869	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	90
3		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	87
4		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5		Carbonic acid, methyl ester, [(E...	280	C17H28O3	1000164-38-7	56



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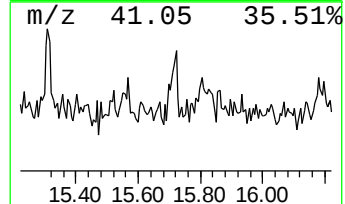
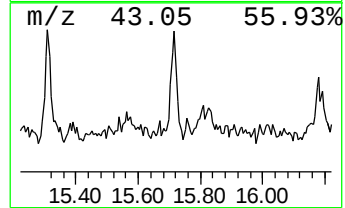
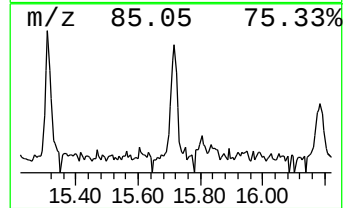
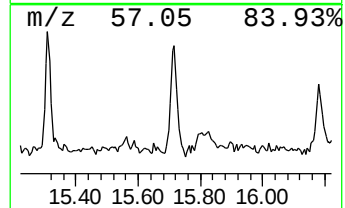
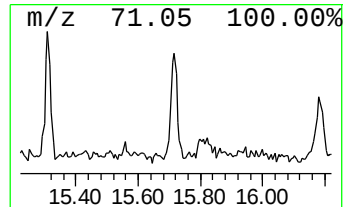
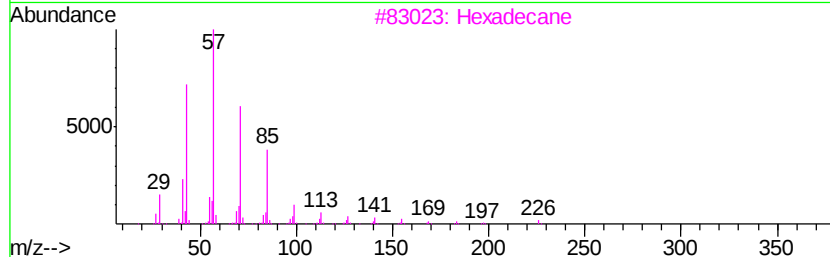
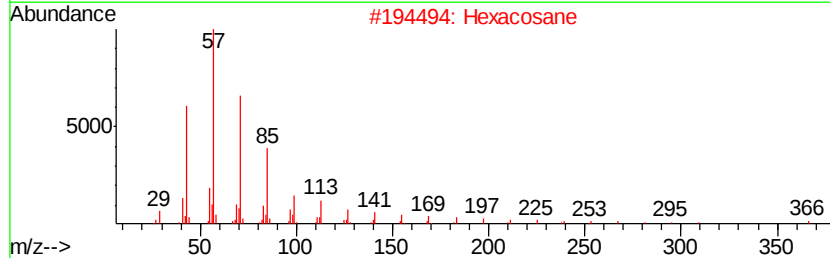
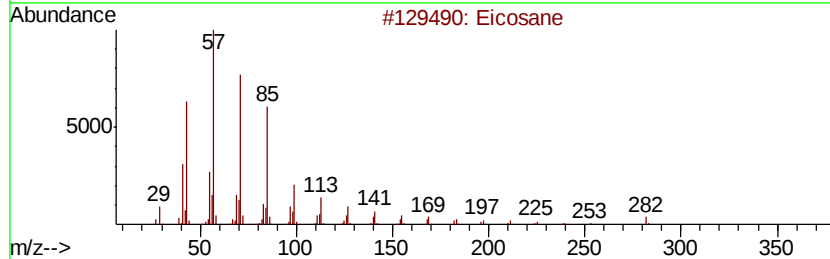
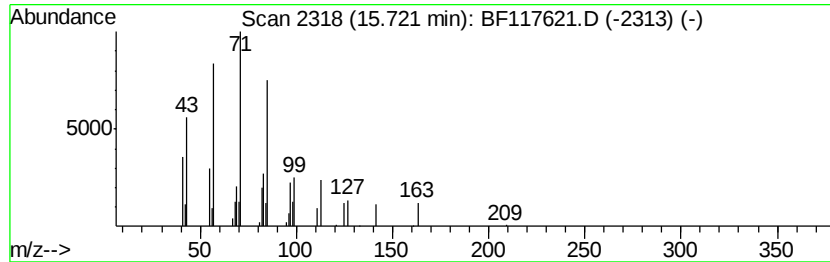
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Peak Number 6 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	2.47 ng	29091	Perylene-d12	15.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	94
2	Hexacosane		366	C26H54	000630-01-3	78
3	Hexadecane		226	C16H34	000544-76-3	78
4	triacontane		422	C30H62	000638-68-6	72
5	Tetracosane		338	C24H50	000646-31-1	72



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Sample : K5539-19
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
165-84-(0-1)

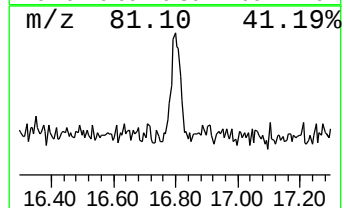
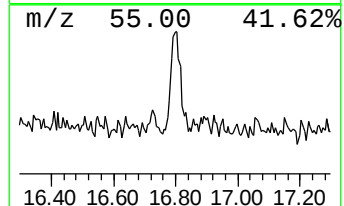
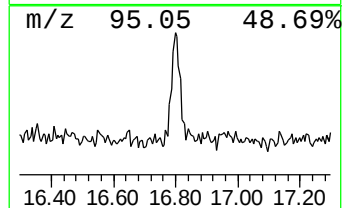
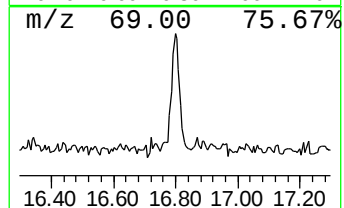
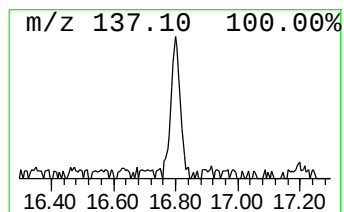
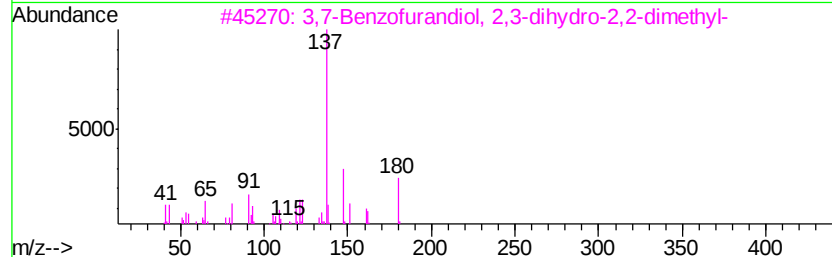
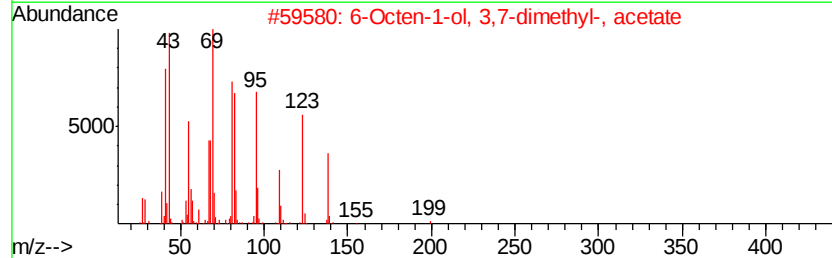
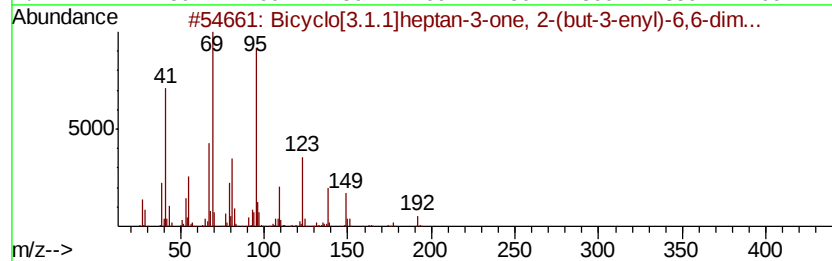
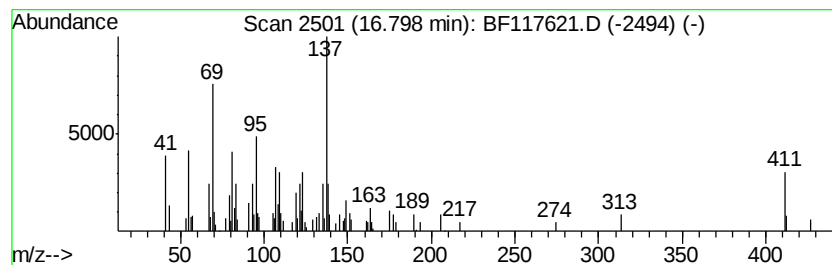
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown16.80 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.80	12.05 ng	141757	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[3.1.1]heptan-3-one, 2-(b...	192	C13H20O	1000163-96-1	35
2		6-Octen-1-ol, 3,7-dimethyl-, ace...	198	C12H22O2	000150-84-5	32
3		3,7-Benzofurandiyl, 2,3-dihydro-...	180	C10H12O3	017781-15-6	27
4		cis,trans-3-Ethylbicyclo[4.4.0]d...	166	C12H22	066660-41-1	27
5		6-Octen-1-ol, 3,7-dimethyl-, for...	184	C11H20O2	000105-85-1	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF103019\
Data File : BF117621.D
Acq On : 30 Oct 2019 13:46
Operator : JU
Sample : K5539-19
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
165-84-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown6.50	6.50	78.7	ng	793440	1	6.73	201538	20.0
Dodecanoic acid	11.77	2.9	ng	37728	4	11.25	257064	20.0
n-Tetracosanol-1	13.73	7.8	ng	96365	5	13.89	248142	20.0
Squalene	14.71	5.4	ng	63869	6	15.33	235370	20.0
Eicosane	15.72	2.5	ng	29091	6	15.33	235370	20.0
unknown16.80	16.80	12.1	ng	141757	6	15.33	235370	20.0